Mechanism for Aqueous Glycine Condensation

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Sanibel Symposium, February, 2008, St. Simons Island, GA, USA

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We investigate the mechanism for aqueous glycine condensation,

$$2\ NH_2CH_2COOH \longrightarrow NH_2CH_2CONHCH_2COOH + H_2O$$

The MP2/6-31G* model chemistry is used to calculate structures and energies of minima and maxima on a reaction coordinate diagram. Results for optimized reactant pair complex, two intermediates, and products are reported. The reactant pair complex had a C-N bond interaction distance of 2.8Å. The first intermediate has a glycylglycine backbone with multiple waters of hydration forming ring-like structures bridging the central carboxylic oxygen atoms with adjacent amine hydrogen atoms, with a C-N bond distance of 1.60Å. The second intermediate has a glycylglycine backbone with two hydroxyl groups on the carbon atom of the incipient peptide bond, and a C-N bond distance of 1.44Å. The product peptide bond distance is 1.37 Å.